DIATOMIC: A POWERFUL SPECTRAL SIMULATION PROGRAM FOR DIATOMIC MOLECULES[a]

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Diatomic is a Windows GUI program that allows user to simulate electronic and infrared spectra of diatomic molecules. Major features of the program include: (i) Multiple coupling schemes are supported: Hund case (a) limit, Hund case (b) limit and intermediate case coupling. (ii) Higher order centrifugal corrections as well as fine structure interactions (spin-orbit, spin-spin and spin-rotation) are included in the frequency calculation. (iii) Λ-type doubling up to Λ=2, S=2 can be included in the frequency calculation. (iv) Calculation of vibrational intensity distribution is supported in simulations involving multiple vibrational bands by constructing RKR potentials from spectroscopic constants and evaluating Franck-Condon factors numerically. (v) Nuclear spin statistics can be taken into account in the intensity calculation. (vi) Effects of excitation-detection geometry, polarization and alignment of the initial-state angular momentum on lines intensities can be taken into account in LIF simulations. (vii) Calculation of line profiles is integrated. Gaussian, Lorentzian and Voigt profiles are supported in LIF simulations; convolution integration of Gaussian or Lorentzian intrinsic profile with instrumental slit transmission function (rectangular or grating diffraction function) is supported in chemiluminescence simulations. (viii) Rotational lines are automatically labeled in simulations. (ix) Graphical tools for spectrum manipulation, magnification and comparison are included. (x) Customized report and printing are supported.

The program is free for research and educational purposes.

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